

Spin- $\frac{1}{2}$ particle in an absorbing environment

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Abstract

The quantum dynamics of a localized spin- $\frac{1}{2}$ Particle interacting with an absorbing environment is investigated. The quantum Langevin-Schrödinger equation for spin- $\frac{1}{2}$ is obtained. The susceptibility function of the environment is calculated in terms of the coupling function of the spin and the environment. it is shown that the susceptibility function satisfies the Kramers-Kronig relations. Spontaneous emission and the shift frequency of the spin is obtained in terms of the imaginary part of the susceptibility function in frequency domain. Some transition probabilities between the spin states are calculated when the absorbing environment is in the thermal state.

1 Introduction

There are mainly two approaches to study dissipative quantum systems. One approach is a phenomenological treatment under the assumption of nonconservative forces[1, 2]. The second approach is found in the interaction between two systems via an irreversible energy flow [3]-[5].

In the frame work of the first approach in studying nonconservative systems, it is essential to introduce a time dependent Hamiltonian which describes the damped motion. Such a phenomenological approach for the study of dissipative quantum systems, specially a damped harmonic oscillator, has a

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rather long history. Caldirola and Kanai [6, 7] adopted a Hamiltonian for a harmonic oscillator so that the Heisenberg equation of the oscillator is identical to the classical equation of a damped harmonic oscillator. The quantum aspect of this model has been studied in a great amount of literature. In those studies some peculiarities of this model and some features of it have appeared to be ambiguous [8]-[16]. There are significant difficulties in obtaining the quantum mechanical solutions for the Caldirola-Kanai Hamiltonian. Quantization with this Hamiltonian violates the uncertainty relations. That is the uncertainty relations vanish as time goes to infinity,[17]-[20]. Based on Caldirola-Kanai Hamiltonian, equivalent theories have been constructed by performing a quantum canonical transformation. Also the path integral techniques has been used to calculate the exact propagators of such theories. The time evolution of a given initial wave functions have been studied using the obtained propagators [21]. In the framework of the phenomenological approach Lopez and Gonzales [22] have taken the external non conservative forces that has linear and quadratic dependence with respect to velocity. They have deduced classical constants of motion and Hamiltonian for these systems. The eigenvalues of these constants have been quantized through perturbation theory.

In the second approach to study quantum dissipative systems one tries to bring about the dissipation as a results of an averaging over all the coordinates of a bath system. One considers the whole system as composed of two parts, our main system and the bath system which interacts with the main system and causes the dissipation of energy on it[23]-[30]. The macroscopic description of a quantum particle with dissipation and moving in an external potential is formulated in terms of the Langevin- Schrödinger equation [31, 32]

$$m\ddot{\vec{x}} + \int_0^t dt' \mu(t-t') \dot{\vec{x}}(t') = -\vec{\nabla}v(\vec{x}) + \vec{F}_N(t) \quad (1)$$

The coupling with the heat-bath in microscopic levels correspond two terms in macroscopic description. A mean force characterized by a memory function $\mu(t)$ and an operator valued random force $\vec{F}_N(t)$. These two terms have a fluctuation-dissipation relation and both are required for a consistent quantum mechanical description of the particle. In [32] there are some models for interaction of the main system with the heat-bath which leads to macroscopic Langevin-Schrödinger equation.

In the present paper we use the second approach for a damped spin- $\frac{1}{2}$ particle

embedded in a uniform magnetic field. In section 2 the absorbing environment of the spin is modeled by a continuous set of harmonic oscillators and quantum dynamics of the spin is investigated. In section 3 the spontaneous emission and the shift frequency of the spin are calculated. In section 4 some transition probabilities between the eigenstates of the spin are computed when the state of the environment is thermal state.

2 Quantum dynamic

Suppose a localized spin- $\frac{1}{2}$ particle is in a constant magnetic field $\vec{B} = B_0 \hat{n}$ along a unit vector \hat{n} and interacts with an absorbing environment. Then the total Hamiltonian can be written as three parts

$$H = H_s + H_{Bs} + H_B \quad (2)$$

H_s is the Hamiltonian of the spin- $\frac{1}{2}$ particle in the constant magnetic field

$$H_s = \omega_0 \vec{S} \cdot \hat{n} \quad (3)$$

where $\omega_0 = \frac{|e|B_0}{mc}$ and e, m are the charge and mass of the particle and c is the speed of light. H_B is the Hamiltonian of the absorbing environment containing a continuum set of harmonic oscillators

$$H_B = \sum_{\lambda=1}^3 \int d^3k \hbar \omega_{\vec{k}} a_{\vec{k}\lambda}^\dagger a_{\vec{k}\lambda} \quad (4)$$

where $\omega_{\vec{k}} = c|\vec{k}|$ and $a_{\vec{k}\lambda}, a_{\vec{k}\lambda}^\dagger$ are annihilation and creation operators of the absorbing environment, respectively and satisfy the commutation relations

$$[a_{\vec{k}\lambda}, a_{\vec{k}'\lambda'}^\dagger] = \delta_{\lambda\lambda'} \delta(\vec{k} - \vec{k}'). \quad (5)$$

In (2) H_{sB} is the interaction part of the spin and the environment and can be proposed as

$$H_{sB} = -\vec{S} \cdot \vec{R} \quad (6)$$

where $\vec{R}(t)$ in the Heisenberg picture is as follows

$$\vec{R}(t) = \sum_{\lambda=1}^3 \int d^3k [f(\omega_{\vec{k}}) a_{\vec{k}\lambda}(t) + f^*(\omega_{\vec{k}}) a_{\vec{k}\lambda}^\dagger(t)] \hat{e}_{\vec{k}\lambda} \quad (7)$$

In this relation $\hat{e}_{\vec{k}\lambda}$ $\lambda = 1, 2, 3$ are three orthogonal unit vectors and $f(\omega_{\vec{k}})$ is called the coupling function between the spin- $\frac{1}{2}$ and the environment and has a crucial role in this theory.

It can be easily shown that the equation of motion of the spin in the Heisenberg picture is obtained as

$$\dot{\vec{S}} = \frac{i}{\hbar}[H, \vec{S}] \Rightarrow \dot{\vec{S}} = \omega(\hat{n} \times \vec{S}) - \vec{R} \times \vec{S} \quad (8)$$

where the commutation relations $[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k$ has been used. Also the Heisenberg equation for the annihilation operators $a_{\vec{k}\lambda}$ are

$$\dot{a}_{\vec{k}\lambda}(t) = -i\omega_{\vec{k}}a_{\vec{k}\lambda}(t) + \frac{i}{\hbar}f^*(\omega_{\vec{k}})\vec{S}(t) \cdot \hat{e}_{\vec{k}\lambda} \quad (9)$$

This equation can be solved formally as

$$a_{\vec{k}\lambda}(t) = a_{\vec{k}\lambda}(0)e^{-i\omega_{\vec{k}}t} + \frac{i}{\hbar}f^*(\omega_{\vec{k}})\hat{e}_{\vec{k}\lambda} \cdot \int_0^t dt' e^{-i\omega_{\vec{k}}(t-t')} \vec{S}(t') \quad (10)$$

substituting $a_{\vec{k}\lambda}(t)$ from (10) in (7) and doing some calculations give us the time dependence of $\vec{R}(t)$ as

$$\vec{R}(t) = \vec{R}_N(t) + \int_0^{|t|} dt' \chi(|t| - t') \vec{S}(\pm t') \quad (11)$$

where the upper (lower) sign is for $t > 0$ ($t < 0$) and $\chi(t)$ is the susceptibility tensor of the absorbing environment and is obtained as

$$\chi(t) = \frac{8\pi}{\hbar c^3} \int_0^\infty d\omega \omega^2 |f(\omega)|^2 \sin \omega t \Theta(t) \quad (12)$$

where $\Theta(t)$ is the step function. The equation (11) may be interpreted the constitutive relation or response equation of the environment. One can be shown that the susceptibility tensor χ satisfies the Kromers-Kronig relations[33]

$$\begin{aligned} Re[\tilde{\chi}(\omega)] &= \frac{2}{\pi} P \int_0^\infty d\omega' \frac{\omega' Im[\tilde{\chi}(\omega')]}{\omega'^2 - \omega^2} \\ Im[\tilde{\chi}(\omega)] &= -\frac{2\omega}{\pi} P \int_0^\infty d\omega' \frac{Re[\tilde{\chi}(\omega')]}{\omega'^2 - \omega^2} \end{aligned} \quad (13)$$

where the symbol P denote the cauchy principal value of the integrals and

$$\tilde{\chi}(\omega) = \int_0^\infty dt \chi(t) e^{i\omega t} \quad (14)$$

is Fourier transformation of $\chi(t)$. In (11) $\vec{R}_N(t)$ is a noise field and is obtained in terms of the annihilation and creation operators of the environment at $t = 0$ as

$$\vec{R}_N(t) = \sum_{\lambda=1}^3 \int d^3k [f(\omega_{\vec{k}}) a_{\vec{k}\lambda}(0) e^{-i\omega_{\vec{k}}t} + f^*(\omega_{\vec{k}}) a_{\vec{k}\lambda}^\dagger(0) e^{i\omega_{\vec{k}}t}] \hat{e}_{\vec{k}\lambda} \quad (15)$$

Finally insertion $\vec{R}(t)$ from (11) into equation (8) leads to the equation of motion of the spin as

$$\dot{\vec{S}} - \omega(\hat{n} \times \vec{S}) + \int_0^{|t|} dt' \chi(|t| - t') (\vec{S}(\pm t') \times \vec{S}(t)) = -\vec{R}_N(t) \times \vec{S}(t) \quad (16)$$

which can be interpreted as the Langevin -Schrödinger equation for the spin in an absorbing environment.

3 Spontaneous emission

In this section the spontaneous decay rate of an initially excited spin- $\frac{1}{2}$ particle is calculated. For simplicity, we assume the spin is in a constant magnetic field along the z axis. Therefore the Hamiltonian (2) can be written as

$$\begin{aligned} H &= H_0 + H' \\ H_0 &= \omega_0 S_z + \sum_{\lambda=1}^3 \int d^3k \hbar \omega_{\vec{k}} a_{\vec{k}\lambda}^\dagger a_{\vec{k}\lambda} \\ H' &= -\vec{S} \cdot \vec{R} \end{aligned} \quad (17)$$

To study the spontaneous emission the interaction picture is used and we apply the Weisskopf-Wigner approximation[34]. The interaction Hamiltonian

H' in interaction picture is as follows

$$\begin{aligned}
H'_I(t) = & - \sum_{\lambda=1}^3 \int d^3k f(\omega_{\vec{k}}) e^{i(\omega_0 - \omega_{\vec{k}})t} \left(\frac{e_{\vec{k}\lambda x}}{2} + \frac{e_{\vec{k}\lambda y}}{2i} \right) a_{\vec{k}\lambda}(0) S_+(0) \\
& - \sum_{\lambda=1}^3 \int d^3k f^*(\omega_{\vec{k}}) e^{i(\omega_{\vec{k}} - \omega_0)t} \left(\frac{e_{\vec{k}\lambda x}}{2} - \frac{e_{\vec{k}\lambda y}}{2i} \right) a_{\vec{k}\lambda}^\dagger(0) S_-(0)
\end{aligned} \tag{18}$$

where the rotating -wave approximation [34] has been used and $S_+ = S_x + iS_y$, $S_- = S_x - iS_y$. In the framework of the Weisskopf-Wigner theory the wave function of the total system in interaction picture is written as

$$|\psi(t)\rangle_I = c(t) \left| \frac{\hbar\omega}{2} \right\rangle_s |0\rangle_R + \sum_{\mu=1}^3 \int d^3q D_{q\mu}(t) \left| -\frac{\hbar\omega}{2} \right\rangle_s |\vec{q}, \mu\rangle_R \tag{19}$$

where $|0\rangle_R$ and $|\vec{q}, \mu\rangle_R$ are the vacuum state and an excited state of the absorbing environment, respectively. The coefficients $c(t)$ and $D_{\vec{q}\mu}(t)$ should be specified by the Schrödinger equation in interaction picture as

$$H'_I(t) |\psi(t)\rangle_I = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I \tag{20}$$

for initial condition $c(0) = 1$, $D_{\vec{q}\mu}(0) = 0$. Substituting $|\psi(t)\rangle_I$ from (19) into (20) and applying $H'_I(t)$ into (18) leads to the following coupled differential equations for the coefficients $c(t)$ and $D_{\vec{q}\mu}(t)$

$$i\hbar \dot{c}(t) = -\hbar \sum_{\lambda=1}^3 \int d^3k f(\omega_{\vec{k}}) e^{i(\omega_0 - \omega_{\vec{k}})t} \left(\frac{e_{\vec{k}\lambda x}}{2} + \frac{e_{\vec{k}\lambda y}}{2i} \right) D_{\vec{k}\lambda}(t) \tag{21}$$

$$i\hbar \dot{D}_{\vec{k}\lambda}(t) = -\hbar f^*(\omega_{\vec{k}}) e^{i(\omega_{\vec{k}} - \omega_0)t} \left(\frac{e_{\vec{k}\lambda x}}{2} - \frac{e_{\vec{k}\lambda y}}{2i} \right) c(t) \tag{22}$$

Integrating equation (22), one can find the coefficient $D_{\vec{k}\lambda}(t)$ in terms of $c(t)$ as

$$D_{\vec{k}\lambda}(t) = f^*(\omega_{\vec{k}}) \int_0^t dt' e^{i(\omega_{\vec{k}} - \omega_0)t'} c(t') \left[\frac{ie_{\vec{k}\lambda x}}{2} - \frac{e_{\vec{k}\lambda y}}{2} \right] \tag{23}$$

where the initial condition $D_{\vec{k}\lambda}(0) = 0$ has been used. Now substituting $D_{\vec{k}\lambda}(t)$ from (23) in (21) and using the completeness relation $\sum_{\lambda=1}^3 e_{\vec{k}\lambda i} e_{\vec{k}\lambda j} =$

δ_{ij} gives us the following integro- differential equation for $c(t)$

$$\dot{c}(t) = \int_0^t dt' \gamma(t-t') c(t') \quad (24)$$

where

$$\gamma(t-t') = -\frac{1}{2} \int d^3k |f(\omega_{\vec{k}})|^2 e^{i(\omega_0 - \omega_{\vec{k}})(t-t')} \quad (25)$$

Here we restrict our attention to the weak-coupling regime where the Markov approximation applies and replace $c(t')$ in integrand (24) by $c(t)$. Also we estimate the integral $\int_0^t dt' e^{i(\omega_0 - \omega_{\vec{k}})(t-t')}$ for sufficiently long time as [35]

$$\int_0^t dt' e^{i(\omega_0 - \omega_{\vec{k}})(t-t')} \simeq iP \frac{1}{\omega_0 - \omega_{\vec{k}}} + \pi \delta(\omega_0 - \omega_{\vec{k}}) \quad (26)$$

where P denotes the cauchy principal value. Finally combination of the relations (24), (25) and (26) leads to

$$\dot{c}(t) = -(\beta + i\Delta) c(t) \quad (27)$$

where

$$\beta = \frac{2\pi^2}{c^3} \omega_0^2 |f(\omega_0)|^2 = \frac{\hbar}{2} \text{Im}[\tilde{\chi}(\omega_0)] \quad (28)$$

is the decay rate of spontaneous emission of an initially excited spin- $\frac{1}{2}$ and

$$\Delta = \frac{2\pi}{c^3} P \int_0^\infty d\omega' \frac{\omega'^2 |f(\omega')|^2}{\omega_0 - \omega'} = \frac{\hbar}{2\pi} \int_0^\infty d\omega' \frac{\text{Im}[\tilde{\chi}(\omega')]}{\omega_0 - \omega'} \quad (29)$$

is the shift frequency.

4 Transition probabilities

In this section we find some transition probabilities between eigen states of $\omega_0 S_z$, when the absorbing environment is in thermal state $\rho_B^T = \frac{e^{-\frac{H_B}{KT}}}{\text{Tr}_B(e^{-\frac{H_B}{KT}})}$, where K is Boltzmann constant and Tr_B denotes tracing over the degrees of freedom of the environment. In order to obtain transition probabilities, we find the density operator of the total system in interaction picture using the perturbation theory. The time evolution of the density operator of the total system in interaction picture can be obtained as

$$\rho_I(t) = U_I^\dagger(t) \rho_I(0) U_I(t) \quad (30)$$

where $U_I(t)$ is the time-evolution operator in interaction picture and up to the first order perturbation is as

$$U_I(t) = 1 - \frac{i}{\hbar} \int_0^t dt_1 H'_I(t_1) \quad (31)$$

Substituting $H'_I(t)$ from (18) in (31) leads to

$$\begin{aligned} U_I(t) = & 1 - \frac{i}{\hbar} \left[- \sum_{\lambda=1}^3 \int d^3k f(\omega_{\vec{k}}) \left(\frac{e_{\vec{k}\lambda x}}{2} + \frac{e_{\vec{k}\lambda y}}{2i} \right) e^{\frac{i(\omega_0 - \omega_{\vec{k}})t}{2}} \frac{\sin \frac{(\omega_0 - \omega_{\vec{k}})t}{2}}{\frac{(\omega_0 - \omega_{\vec{k}})}{2}} a_{\vec{k}\lambda}(0) S_+(0) \right] \\ & + \frac{i}{\hbar} \left[\sum_{\lambda=1}^3 \int d^3k f^*(\omega_{\vec{k}}) \left(\frac{e_{\vec{k}\lambda x}}{2} - \frac{e_{\vec{k}\lambda y}}{2i} \right) e^{\frac{i(\omega_0 - \omega_{\vec{k}})t}{2}} \frac{\sin \frac{(\omega_0 - \omega_{\vec{k}})t}{2}}{\frac{(\omega_0 - \omega_{\vec{k}})}{2}} a_{\vec{k}\lambda}^\dagger(0) S_-(0) \right] \quad (32) \end{aligned}$$

In order to compute the transition probabilities between eigen states of $\omega_0 S_z$ we need the reduced density operator of the system which is defined by $\rho_{sI}(t) = \text{Tr}_B[\rho_I(t)]$. Let the initial density operator of the total system in interaction picture at $t = 0$ is $\rho_I(0) = |\frac{\hbar\omega_0}{2}\rangle\langle\frac{\hbar\omega_0}{2}| \otimes \rho_B^T$, then the reduced density operator is obtained as

$$\begin{aligned} \rho_{sI}(t) = & |\frac{\hbar\omega_0}{2}\rangle\langle\frac{\hbar\omega_0}{2}| \\ & + \frac{1}{2} \int d^3k |f(\omega_{\vec{k}})|^2 \frac{\sin^2 \frac{(\omega_{\vec{k}} - \omega_0)t}{2}}{(\frac{\omega_0 - \omega_{\vec{k}}}{2})^2} \frac{e^{\frac{\hbar\omega_{\vec{k}}}{KT}}}{e^{\frac{\hbar\omega_{\vec{k}}}{KT}} - 1} |\frac{-\hbar\omega_0}{2}\rangle\langle\frac{-\hbar\omega_0}{2}| \quad (33) \end{aligned}$$

where the completeness relation $\sum_{\lambda=1}^3 e_{\vec{k}\lambda i} e_{\vec{k}\lambda j} = \delta_{ij}$ and

$$\text{Tr}_B[a_{\vec{k}\lambda}^\dagger \rho_B^T a_{\vec{k}'\lambda'}] = \delta(\vec{k} - \vec{k}') \delta_{\lambda\lambda'} \frac{e^{\frac{\hbar\omega_{\vec{k}}}{KT}}}{\frac{\hbar\omega_{\vec{k}}}{KT} - 1} \quad (34)$$

have been used. Now if a measurement is done on the Hamiltonian $\omega_0 S_z$ the probability that the eigenvalue $-\frac{\hbar\omega_0}{2}$ is obtained for sufficiently long times is

$$\Gamma_{|\frac{\hbar\omega_0}{2}\rangle \rightarrow |-\frac{\hbar\omega_0}{2}\rangle} = \text{Tr}_s \left[|-\frac{\hbar\omega_0}{2}\rangle\langle-\frac{\hbar\omega_0}{2}| \rho_{sI}(t) \right] = \hbar t \text{Im}[\tilde{\chi}(\omega_0)] \frac{e^{\frac{\hbar\omega_0}{KT}}}{e^{\frac{\hbar\omega_0}{KT}} - 1} \quad (35)$$

where Tr_s denotes tracing over the degrees of freedom of spin- $\frac{1}{2}$ particle. Now assume the initial density operator of the total system in interaction picture is $\rho_I(0) = |\frac{-\hbar\omega_0}{2}\rangle\langle\frac{-\hbar\omega_0}{2}| \otimes \rho_B^T$. It is easy to show that the reduced density operator of system is

$$\rho_{sI}(t) = |\frac{-\hbar\omega_0}{2}\rangle\langle\frac{-\hbar\omega_0}{2}| + \frac{1}{2} \int d^3k |f(\omega_{\vec{k}})|^2 \frac{\sin^2 \frac{(\omega_{\vec{k}} - \omega_0)t}{2}}{(\frac{\omega_0 - \omega_{\vec{k}}}{2})^2} \frac{1}{e^{\frac{\hbar\omega_{\vec{k}}}{KT}} - 1} |\frac{\hbar\omega_0}{2}\rangle\langle\frac{\hbar\omega_0}{2}| \quad (36)$$

where

$$Tr_B[a_{\vec{k}\lambda} \rho_B^T a_{\vec{k}'\lambda'}^\dagger] = \delta(\vec{k} - \vec{k}') \delta_{\lambda\lambda'} \frac{1}{e^{\frac{\hbar\omega_{\vec{k}}}{KT}} - 1} \quad (37)$$

has been used. A simple calculation shows that in this case if the Hamiltonian $\omega_0 S_z$ is measured the probability that the eigenvalue $\frac{\hbar\omega_0}{2}$ is obtained for very long times is

$$\Gamma_{|\frac{-\hbar\omega_0}{2}\rangle \rightarrow |\frac{\hbar\omega_0}{2}\rangle} = Tr_s \left[|\frac{\hbar\omega_0}{2}\rangle\langle\frac{\hbar\omega_0}{2}| \rho_{sI}(t) \right] = \hbar t Im[\tilde{\chi}(\omega_0)] \frac{1}{e^{\frac{\hbar\omega_0}{KT}} - 1} \quad (38)$$

From this transition probability it is clear that at very low temperature $\Gamma_{|\frac{-\hbar\omega_0}{2}\rangle \rightarrow |\frac{\hbar\omega_0}{2}\rangle}$ tends to zero.

5 Summary and conclusion

The absorbing environment of a spin- $\frac{1}{2}$ particle is modeled by a continuum set of harmonic oscillators. A coupling function is introduced that couple the spin and the environment. A susceptibility function is attributed to the environment that is obtained in terms of the coupling function. It was shown that the susceptibility function satisfies the Kramers-Kronig relations as in electrodynamics. The quantum Langevin-Schrödinger equation is obtained as equation of motion of the spin in Heisenberg picture. It is assumed that the spin is in a uniform external magnetic field along the z axis and spontaneous emission of the spin is calculated in the presence of the absorbing environment. The spontaneous emission and the shift frequency of the spin is obtained in terms of the imaginary part of the susceptibility function of the environment in frequency domain. Some transition probabilities between eigen states of the spin (embedded in the uniform magnetic field) is computed

when the environment is in thermal state. It is shown when the temperature of the environment tends to zero there exist an irreversible current of energy from the spin to the environment.

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